Nuclear Structure Calculations with Low-Momentum Potentials in a Model Space Truncation Approach

L. Coraggio,[1] A. Covello,[1] A. Gargano,[1] N. Itaco,[1] and T. T. S. Kuo[2]

[1] *Dipartimento di Scienze Fisiche, Università di Napoli Federico II, and Istituto Nazionale di Fisica Nucleare, Complesso Universitario di Monte S. Angelo, Via Cintia - I-80126 Napoli, Italy*

[2] *Department of Physics, SUNY, Stony Brook, New York 11794*

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We have calculated the ground-state energy of the doubly magic nuclei ^{4}He, ^{16}O and ^{40}Ca within the framework of the Goldstone expansion starting from various modern nucleon-nucleon potentials. The short-range repulsion of these potentials has been renormalized by constructing a low-momentum potential $V_{\rm low-k}$. We have studied the connection between the cutoff monemtum Λ and the size of the harmonic oscillator space employed in the calculations. We have found a fast convergence of the results with a limited number of oscillator quanta.

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I. INTRODUCTION

One of the well-known important features of realistic nucleon-nucleon (NN) potentials is their strong repulsive behavior in the high-momentum regime. This implies that when performing nuclear structure calculations within a perturbative approach it is unavoidable to renormalize the NN potential. The renormalization may be achieved by constructing a potential that takes into account the high momentum components of the original potential in an effective way. For example, the well-known Brueckner reaction matrix G [1] is an energy-dependent effective interaction, defined in a model space P, obtained projecting out all two-particle excitations above a chosen Fermi surface. The main drawback of such a procedure is that the G matrix is energy dependent, which stems from the fact that it does not fulfill a decoupling condition between the model space P and its complement Q.

Recently, we have proposed [2, 3] a new method to renormalize the bare NN interaction, which is proving to be an advantageous alternative to the use of the Brueckner G matrix. We define a low-momentum P-space up to a cutoff momentum Λ and derive from the original V_{NN} an effective low-momentum potential $V_{\rm low-k}$ that satisfies the decoupling condition between the low- and high-momentum spaces. This $V_{\rm low-k}$ is a smooth potential which preserves exactly the on-shell properties of the original V_{NN} and is suitable for being used directly in nuclear structure calculations.

In applying the low-momentum NN potential $V_{\rm low-k}$ to nuclear structure calculations, an important step is the determination of the decimation momentum Λ for $V_{\rm low-k}$. There are two considerations: first, Λ is based on the separation of scale idea of the renormalization-group effective field theory (RGEFT) approach. In low-energy nuclear physics, one is interested in phenomena at low-energy scale and consequently the details of the short-distance (high-energy scale) physics are unimportant. This leads to the derivation of the low-momentum potential $V_{\rm low-k}$ by integrating out the high-momentum components of modern NN potentials beyond a cutoff momentum Λ.

The second consideration is that all modern NN potentials are constructed to fit the empirical phase shifts up to the inelastic threshold $E_{\rm lab} \simeq 350$ MeV, which corresponds to a maximum relative momentum $\simeq 2.1$ fm^{-1}.

In the past few years, we have profitably employed this technique in realistic nuclear structure calculations for both doubly closed-shell nuclei, within the framework of the Goldstone expansion [4, 5], and open-shell nuclei within the multilevel shell-model framework [2, 3, 6, 7, 8]. In all these works we have used for the cutoff momentum the value $\Lambda = 2.1$ fm^{-1}.

It is interesting, however, to investigate the relation of the cutoff momentum Λ to the dimension of the configuration space in the coordinate representation, where actually our calculations are performed. The study of such a relation is the aim of the present work, where we show how the choice of a cutoff momentum implies a maximum value for the energy of the two-nucleon system, the latter introducing a simple criterion to choose the two-nucleon model space.

To verify the reliability of this approach we calculate, in the framework of the Goldstone expansion, the ground state (g.s.) properties of doubly closed-shell nuclei starting from different NN potentials renormalized through the $V_{\rm low-k}$ procedure.

The paper is organized as follows. In Sec. II we give an outline of our calculations. A detailed discussion of the convergence properties of the perturbative calculations is presented in Sec. III. Sec. IV is devoted to the presentation and discussion of our results for the three nuclei ^{4}He, ^{16}O, and ^{40}Ca. Some concluding remarks are given in Sec. V.

II. OUTLINE OF CALCULATIONS

As already mentioned in the Introduction, we renormalize the short-range repulsion of the bare NN potential V_{NN} by integrating out its high momentum components through the so-called $V_{\rm low-k}$ approach. A detailed description of this procedure can be found in Refs. [3, 9]. The renormalized NN potential $V_{\rm low-k}$ preserves the observables predicted by V_{NN} for the two-nucleon system, and consequently its $\chi^2/datum$, up to the cutoff momentum Λ. The $V_{\rm low-k}$ is a smooth potential and can be used directly in nuclear structure calculations within a perturbative approach.

While the $V_{\rm low-k}$ is defined in the momentum space, we perform our calculations for finite nuclei in the coordinate space employing a truncated harmonic oscillator (HO) basis. Since the $V_{\rm low-k}$ procedure decouples the momentum space into the low- and high-momentum regime, it is desirable to recover such a decoupling in the HO space.

Let us consider the relative motion of two nucleons in a harmonic oscillator well in the momentum representation. For a given maximum relative momentum Λ, the corresponding maximum value of the energy is:

$$E_{\rm max} = \frac{\hbar^2\Lambda^2}{M} \quad , \tag{1}$$

where M is the nucleon mass.

This relation may be re-written in terms of the maximum number $N_{\rm max}$ of HO quanta for the relative coordinate system, so for a given HO parameter $\hbar\omega$ we have:

$$\left(N_{\rm max} + \frac{3}{2}\right)\hbar\omega = \frac{\hbar^2\Lambda^2}{M} \quad . \tag{2}$$

The above equation provides a simple criterion to map out the two-nucleon HO model space. If we write the two-nucleon states as the product of HO wave functions

$$|a\ b\rangle = |n_a l_a j_a,\ n_b l_b j_b\rangle \quad , \tag{3}$$

our HO model space is defined as spanned by those two-nucleon states that satisfy the constraint

$$2n_a + l_a + 2n_b + l_b \leq N_{\rm max} \quad . \tag{4}$$

The need for such a boundary condition for our model space may be also pointed out by the following considerations. The momentum contents of the two-nucleon wave function clearly depend on the choice of the model space. For example, the average momentum of HO wave functions is proportional to $(\hbar\omega)^{1/2}$. Suppose we are doing a calculation using a small model space together with a small $\hbar\omega$, so that the momentum contents of the basis wave functions are practically all below 1.5 fm^{-1}. In this case, we clearly should use this value for Λ. Let us consider another situation where the model-space wave functions have important momentum components of, say, up to 3.0 fm^{-1}. Then in this case, we need to use a larger Λ.

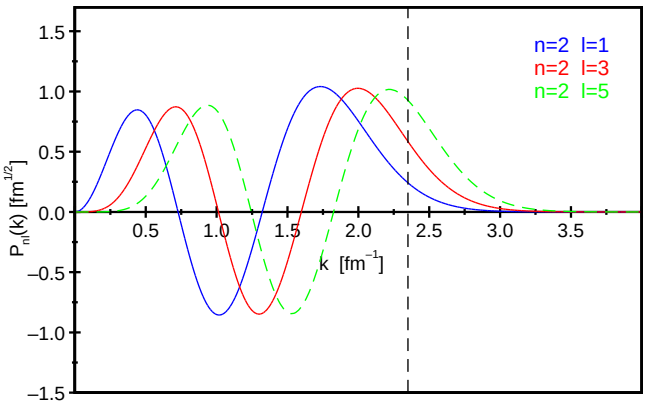

FIG. 1: Different P_{nl}'s for $\hbar\omega$=27 MeV. See text for details.

The above considerations may be illustrated by inspecting the explicit expression of the $V_{\rm low-k}$ matrix elements in terms of wave functions of the center-of-mass and relative coordinates:

$$\langle n_a l_a j_a, n_b l_b j_b; JT|V_{\rm low-k}|n_c l_c j_c, n_d l_d j_d; JT\rangle = \sum_{LL'S} (-1)^{L+L'}$$
$$\hat{j}_a\hat{j}_b\hat{j}_c\hat{j}_d(2L+1)(2L'+1)(2S+1) \left\{ \begin{array}{ccc} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L & S & J \end{array} \right\} \left\{ \begin{array}{ccc} l_c & \frac{1}{2} & j_c \\ l_d & \frac{1}{2} & j_d \\ L' & S & J \end{array} \right\}$$
$$\sum_{nln'l'N\mathcal{L}} [1-(-1)^{l+S+T}] \langle nlN\mathcal{L},\ L|n_a l_a n_b l_b,\ L\rangle$$
$$\langle n'l'N\mathcal{L},\ L'|n_c l_c n_d l_d,\ L'\rangle \sum_{\mathcal{J}} (2\mathcal{J}+1) \left\{ \begin{array}{ccc} \mathcal{L} & l & L \\ S & J & \mathcal{J} \end{array} \right\} \left\{ \begin{array}{ccc} \mathcal{L} & l' & L' \\ S & J & \mathcal{J} \end{array} \right\}$$
$$\langle nlST\mathcal{J}|V_{\rm low-k}|n'l'ST\mathcal{J}\rangle \quad , \tag{5}$$

where $\hat{j} = \sqrt{2j+1}$, $\langle nlN\mathcal{L},\ L|n_a l_a n_b l_b,\ L\rangle$ are the Brody-Moshinsky transformation brackets [10], and, according to (4), $2n+l$ and $2n'+l'$ are both $\leq N_{\rm max}$. The matrix element $\langle nlST\mathcal{J}|V_{\rm low-k}|n'l'ST\mathcal{J}\rangle$ is expressed in terms of the momentum-space HO wave functions P_{nl}'s as

$$\langle nlST\mathcal{J}|V_{\rm low-k}|n'l'ST\mathcal{J}\rangle = \int_0^\Lambda \int_0^\Lambda dk\ dk'\ kk'\ P_{nl}(k)$$
$$P_{n'l'}(k') V^{ll'ST\mathcal{J}}_{\rm low-k}(k,k') \quad . \tag{6}$$

Because in Eq. (6) the integrals are evaluated up to Λ, it is desirable to throw away those P_{nl}'s which extend significantly above the cutoff momentum, and pertain therefore to the high-momentum regime. We have verified that applying the constraint (4) amounts to neglect all P_{nl}'s which extend their tail more than $\simeq 5\%$

above Λ. Fig. 1 is an explanatory picture where we plot, for a given $\hbar\omega$ =27 MeV, three momentum space HO wave functions P_{nl}'s with $2n + l$ =5 , 7, and 9, respectively, as functions of k. The vertical dashed line denotes a value of $\Lambda = 2.35$ fm^{-1}, corresponding to $N_{\max}$=7.

Relation (4) has a general validity, it should be applied every time the $V_{\rm low-k}$ matrix elements are calculated in the HO basis.

In this paper, making use of the present approach, we have studied the ground state properties of doubly closed-shell nuclei within the framework of the Goldstone expansion [11]. More explicitly, starting from the purely intrinsic hamiltonian

$$H = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{p_i^2}{2M} + \sum_{i<j} \left(V_{ij} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{MA}\right) \quad , \qquad (7)$$

where V_{ij} stands for the renormalized V_{NN} potential plus the Coulomb force, we construct the Hartree-Fock (HF) basis expanding the HF single particle (SP) states in terms of HO wave functions. The HF basis is then employed to sum up the Goldstone expansion, including contributions up to fourth-order in the two-body interaction.

Our calculations are made in a truncated model space, whose size is related to the values of the cutoff momentum Λ and the $\hbar\omega$ parameter. The calculations are performed increasing the $N_{\max}$ value (and consequently Λ) and varying the $\hbar\omega$ value until the dependence on $N_{\max}$ (Λ) is minimized.

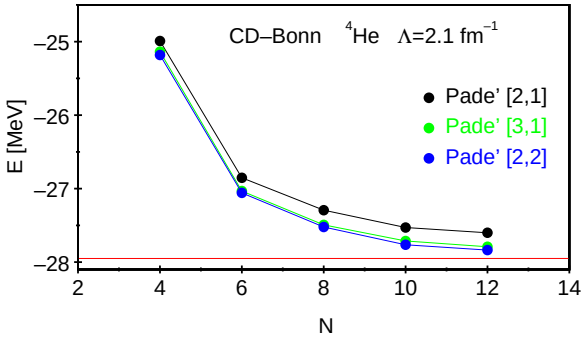

FIG. 2: ^{4}He ground state energy as a function of the number of harmonic-oscillator major shells. The employed two-body interaction is a $V_{\rm low-k}$ derived from CD-Bonn potential with $\Lambda = 2.1$ fm^{-1}. The oscillator parameter $\hbar\omega$ is equal to 18 MeV. Calculations have been performed with different Padé approximants, the red line representing an exact calculation. [15].

III. CONVERGENCE PROPERTIES OF THE PERTURBATIVE EXPANSION

In section IV we will show the calculated ground state energies of some doubly closed-shell nuclei within the framework of the perturbative approach (Goldstone expansion). Here, we study the convergence properties of the perturbative series. To this end, we have performed a test calculation, starting from a $V_{\rm low-k}$ with a fixed cutoff momentum $\Lambda = 2.1$ fm^{-1} and derived from the NN CD-Bonn potential [12]. For this $V_{\rm low-k}$, hermitized according to the procedure based on the Cholesky decomposition suggested in Ref. [13], an exact calculation of the ground state energy of ^{4}He has been performed in the framework of the hyperspherical harmonic (HH) approach [14]. The value obtained is -27.95 MeV [15], considering the $V_{\rm low-k}$ as a NN potential defined in the whole momentum space, with $V_{\rm low-k}(k, k') = 0$ when k or $k' > \Lambda$. With the above potential we have calculated the same quantity in the framework of the Goldstone expansion.

Using Padé approximants [16, 17] one may obtain a value to which the perturbation series should converge. We consider the following three Padé approximants:

$$[L|1] = E_0 + E_1 + ... + \frac{E_L}{1 - E_{L+1}/E_L} \quad , \qquad (8)$$

where $L = 2,\ 3$, and

$$[2|2] = \frac{E_0(1 + \gamma_1 + \gamma_2) + E_1(1 + \gamma_2) + E_2}{1 + \gamma_1 + \gamma_2} \quad , \qquad (9)$$

where

$$\gamma_1 = \frac{E_2 E_4 - E_3^2}{E_1 E_3 - E_2^2} \quad , \qquad \gamma_2 = -\frac{E_3 + E_1\gamma_1}{E_2} \quad ,$$

E_i being the ith order energy contribution in the Goldstone expansion.

In Fig. 2 the ^{4}He calculated ground state energy is plotted versus the number of HO major shells included in the calculation, the red line representing the exact value. It is worth here to mention that no further truncation for the two-nucleon states has been performed, we considering the $V_{\rm low-k}$ as defined in the whole momentum space.

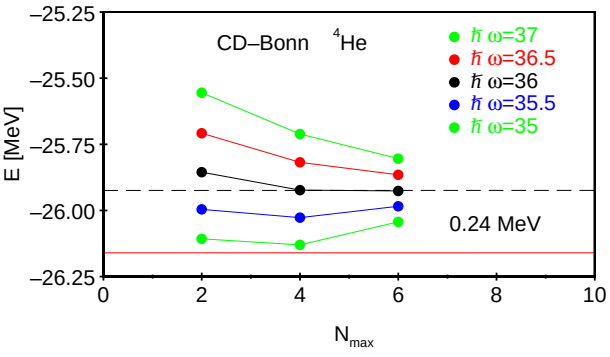

FIG. 3: ^{4}He ground state energy with CD-Bonn potential as function of $N_{\max}$, for different values of $\hbar\omega$. The straight line represents the Faddeev-Yakubovsky result.

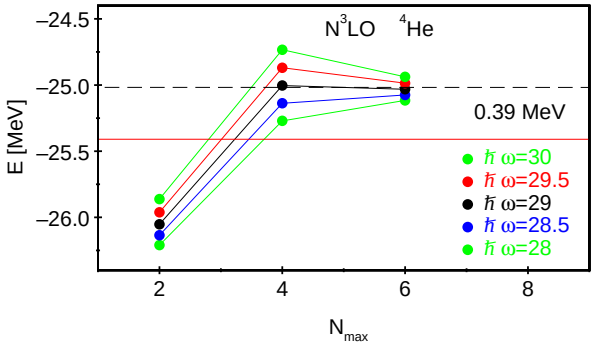

FIG. 4: Same as Fig.3, but for N^{3}LO potential.

We see that the Padé approximants [3|1] and [2|2] give, for a given number of HO major shells, almost the same value , the difference being at most 45 keV. The Padé approximant [2|1] differs at most by 200 keV from the [3|1], and 245 keV from the [2|2]. Moreover, the results, corresponding to the largest space we have employed, come close to the exact value, the energies being -27.79 and -27.84 MeV with the [3|1] and [2|2] approximants, respectively.

On these grounds, we report in the following section the results obtained using the Padé approximant [2|2].

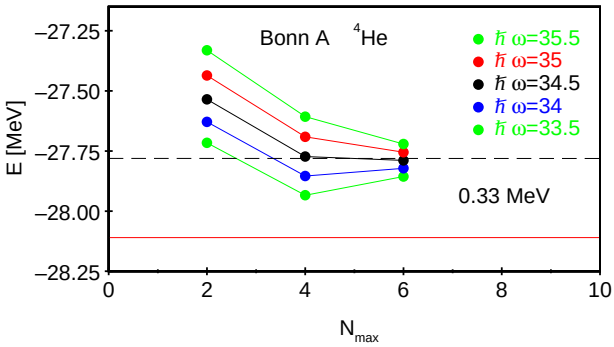

FIG. 5: Same as Fig.3, but for Bonn A potential.

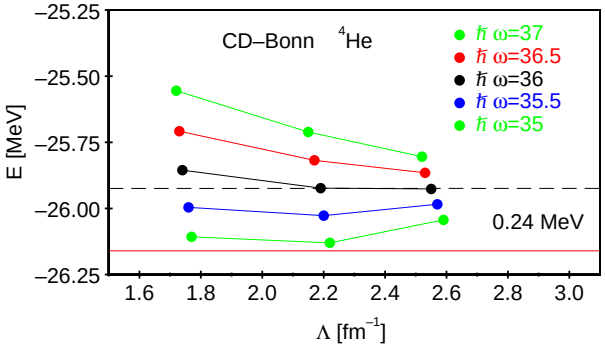

FIG. 6: ^{4}He ground state energy with CD-Bonn potential as function of cutoff momentum Λ, for different values of $\hbar\omega$. The straight line represents the Faddeev-Yakubovsky result.

IV. RESULTS

To test the reliability of our calculations we have calculated the binding energy of ^{4}He starting from different V_{NN}'s, and compared our results with those obtained through the Faddeev-Yakubovsky (FY) method.

In Figs. 3, 4, and 5 we show the calculated ^{4}He ground state energies obtained from the CD-Bonn [12], N^{3}LO [18], and Bonn A [19] NN potentials, respectively. In each figure the straight red line indicates the FY result [20, 21] while the other curves represent our calculated values, for different values of $\hbar\omega$, versus the maximum number of HO quanta $N_{\max}$ that binds the two-nucleon configurations according to the relation (4). In Fig. 6, we report the same results of Fig. 3, but versus the cutoff momentum Λ.

For the CD-Bonn, N^{3}LO, and Bonn A potentials we obtain convergence with $\hbar\omega$ = 36, 29, and 34.5 MeV, respectively. Our calculated energies are -25.92, -25.02, and -27.78 MeV for the above V_{NN}'s. These values are in good agreement with the FY results, the largest discrepancy being 0.39 MeV for N^{3}LO potential. We have done similar calculations starting from other modern NN potentials, such as the Nijmegen II [22] and Argonne V18 [23] potentials, but because of their stronger tensor components it has not been possible to achieve convergence.

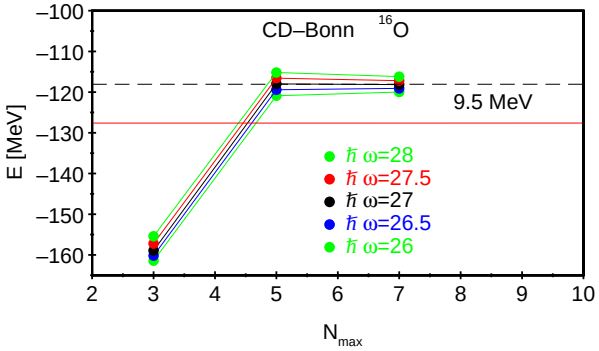

FIG. 7: ^{16}O ground state energy with CD-Bonn potential as function of $N_{\max}$, for different values of $\hbar\omega$. The straight line represents the experimental value [25].

We have calculated also the ground state energies of ^{16}O and ^{40}Ca starting from the CD-Bonn potential. In Fig. 7 we present our results for ^{16}O and compare them with the experimental datum. The converged value, as can be seen from the figure, is obtained for $\hbar\omega$ = 27 MeV and is equal to -118.1 MeV, the discrepancy with the experimental value being 9.5 MeV. In this case we cannot compare our calculations with the exact ones. It is worth mentioning, however, the work by Fujii et al. [24] who, using the unitary model-operator approach (UMOA), predict for the CD-Bonn potential a converged value of -115.61 MeV, including only two-body correlations. In a more recent paper [26], the above authors have estimated the three-body cluster effect to contribute about -4 MeV.

As regards ^{40}Ca, a calculation of its ground state energy including fourth-order contributions in the Goldstone expansion has not been done because of the large CPU time needed. We therefore report in Fig. 8 the results obtained with the Padé approximant [2|1], taking into account up to third-order contributions in the Goldstone expansion. The converged value is -307.8 MeV with $\hbar\omega = 25.5$ MeV. In this case, the discrepancy with respect to the experimental value is 34.2 MeV.

V. SUMMARY

In this work, we have calculated the ground state energy of some doubly closed-shell nuclei in the framework of the Goldstone expansion, starting from different realistic NN potentials. The short-range repulsion of these potentials has been renormalized by integrating out their high-momentum components through the so-called $V_{\rm low-k}$ approach. We have introduced a criterion to map out the model space made up by the two-nucleon states in the HO basis, according to the value of the cutoff momentum Λ.

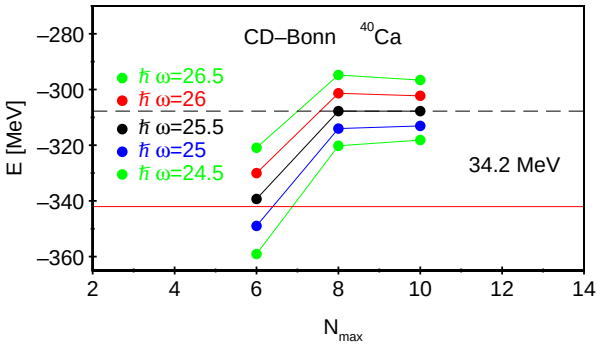

FIG. 8: Same as Fig.7, but for for ^{40}Ca

The reliability of this procedure has been tested by calculating the ground state energy of ^{4}He, with the CD-Bonn, N^{3}LO, and Bonn A potentials and comparing the results with the FY ones. We have found that the energy differences are at most 390 keV. These differences are due to two reasons. On the one hand, our calculations have been performed using a perturbative approach, so that small contributions coming from higher order terms may have not been completely taken into account by the Padé approximants. On the other hand, we do not expect that Eq. (2) recovers exactly in the HO basis the $V_{\rm low-k}$ decoupling into low- and high-momentum regime.

In any case, the limited size of the discrepancies shows that our approach provides a reliable way to renormalize the NN potentials preserving not only the two-body but also the many-body physics.

On the above grounds, we have performed similar calculations for heavier systems, such as ^{16}O and ^{40}Ca and obtained converged results using model spaces not exceeding $N_{\rm max} = 10$.

The rapid convergence of the results with the size of the HO model space makes it very interesting to study in a near future heavier systems employing our present approach.

Acknowledgments

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